

Manuscript submitted to  
AIMS' Journals  
Volume **X**, Number **0X**, XX **200X**

Website: <http://AIMSciences.org>

pp. **X–XX**

## INTERACTION OF MOVING DISCRETE BREATHERS WITH INTERSTITIAL DEFECTS

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**ABSTRACT.** In this paper, interstitial migration generated by scattering with a mobile breather is investigated numerically in a Frenkel-Kontorova one-dimensional lattice. Consistent with experimental results it is shown that interstitial diffusion is more likely and faster than vacancy diffusion. Our simulations support the hypothesis that a long-range energy transport mechanism involving moving nonlinear vibrational excitations may significantly enhance the mobility of point defects in a crystal lattice.

**1. Introduction.** The Frenkel–Kontorova (FK) model, introduced almost 70 years ago [1], is one of the most paradigmatic nonlinear systems, whose dynamics has been widely studied during the last decades (see [2, 3, 4, 5] and references therein). From the point of view of condensed matter physics, its paramount importance relies on the ability to describe a vast number of phenomena, including different kinds of defects such as vacancies (Schottky defects) and, to some extent, interstitials (Frenkel defects), which can play an important role in the design of new materials [6].

As the FK model is basically a one-dimensional lattice of particles subjected to a nonlinear periodic substrate potential and a nearest-neighbour interaction, it contains the basic ingredients to sustain localized excitations such as topological solitons (kinks or antikinks) or breathers. Discrete breathers (DBs), also called intrinsic localized modes (for a very recent review about their properties, existence proofs, computational methods and applications see [7]), are exact solutions of the dynamical equations whose energy, in contrast with normal extended wave excitations, is not shared among lattice components but extends only over a few lattice sites. In this sense, their spatial profiles resembles localized vibrational modes induced by a defect site in a harmonic lattice [8]. However DBs arise only thanks to the interplay between nonlinearity and discreteness and, for that reason, they may occur anywhere in the lattice given sufficient vibrational amplitude. They are also rather universal since they are not specific to Hamiltonians with a particular form and can be found in lattices of arbitrary dimensions. Moreover, theoretical studies

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2000 *Mathematics Subject Classification.* Primary: 70K75, 74J30; Secondary:  
*Key words and phrases.* Moving breathers, kinks, defects, Frenkel–Kontorova model.

have shown DBs are linearly stable [9], which implies they can persist over very long times on top of a thermalized background [10]. Their investigation is not restricted to simple toy models. Apart from indirect spectroscopic observations [11], DBs have been detected and studied experimentally in such different macroscopic systems as waveguide arrays [12], micromechanical cantilevers [13], antiferromagnetic structures [14] and Josephson-junctions [15].

In this context, an interesting problem that has attracted much attention in recent years is the interaction between a moving localized excitation and a lattice defect. The problem has been addressed within different frameworks: impurities [16, 17], lattice junctions [18, 19], bending points of a polymer chain [20, 21, 22], but most studies assume that the position of the defect is fixed and is not able to move along the lattice. Of current interest is the interaction between lattice defects and moving localized excitations, which might result in movement of the defect. This is especially true in the case of interactions arising during irradiation of solids by swift particles, which usually involve the creation of DBs of either longitudinal or transverse optical mode type.

The possibility of such interactions arose in the study of high energy charged particles passing through crystals of muscovite, when scattering events were postulated to create many moving highly energy DBs. It was suggested that when such DBs (there called quodons) reached the end of a chain, which represents a defect in a chain, it might cause the last atom to be ejected from the surface [23]. This prediction was supported by studies using both mechanical and numerical models [24]. Subsequently, it was verified by experiment using a natural crystal of muscovite [25]. In the experiment one edge of a crystal was bombarded with alpha particles at near grazing incidence to create moving DBs. These propagated in chain directions in the layered crystal and caused a proportionate ejection of atoms from a remote edge of the crystal that was  $> 10^7$  unit cells distance in a chain direction from the site of bombardment. As this experiment was performed at 300K it not only verified the prediction but also demonstrated the stability of these mobile DBs against thermal motion.

Other irradiation studies have provided more empirical signs for the interaction of DBs with defects. For instance, in ref. [26] the authors provide evidence that, after irradiating a silicon crystal with silver ions, a pileup of lattice defects is accomplished at locations spatially separated from the irradiation site. The evidence indicated that defects could be swept by up to about 1 micron from the irradiated region. This effect was ascribed to the propagation of highly localized packets of vibrational energy, or DBs, created by the bombardment of heavy ions.

Another ion-induced, athermal transport process was reported in ref. [27]. In this case interstitial N diffusion in austenitic stainless steel under Ar ion bombardment was investigated. It was found that N mobility increases in depths several orders of magnitude larger than the ion penetration depth. This irradiation-induced enhancement of N diffusion is consistent with previous observations which show a dependence of the nitriding depth on ion energy [28] and also on the crystalline orientation [29], but no conventional mechanism of diffusion can explain them. For this reason it was suggested that diffusion of interstitial atoms might be assisted by highly anharmonic localized excitations which propagate distances well beyond the ion penetration depth.

Interstitial atoms reside in potential wells between the lattice atoms. When a breather propagates it strongly disturbs the lattice locally. If it passes near an

interstitial these oscillatory motions will distort the potential well confining the interstitial and will affect significantly its mobility. Interstitial motion consists of jumps from one potential well to the next. Since experimental measures deal with concentration depth profiles, interstitial diffusion process can be analyzed in terms of an effective movement along a one-dimensional chain of potential wells. Moreover the presence of an interstitial modifies potentials in adjacent atomic chains, causing the spacing between the two nearest atoms in a chain to the interstitial to increase. Therefore, in a first approximation, an interstitial can be modelled introducing an additional particle in a one-dimensional system and this provides the link to the FK model.

In this paper, using a FK model with nonlinear nearest-neighbour interaction, it is shown that migration of the disturbance in a chain caused by an interstitial can be induced by scattering with a mobile longitudinal mode breather. Comparison with previous work on vacancies migration [30, 31] also suggests that, according to experimental results, interstitial mobility is more likely and faster than that of vacancy defects. Of course, the specific constraints of a one-dimensional system implies that care is needed when attempting to carry over results to higher dimensional lattices. Nevertheless we think that a one-dimensional study is a necessary and useful first step before approaching the problem with a more realistic and complex two or three-dimensional model.

**2. The model.** As described in the introduction, the F-K model consists of a chain of interacting particles subject to a periodic substrate potential. This system is described by the following Hamiltonian:

$$H = \sum_{n=1}^N \frac{1}{2} m \dot{x}_n^2 + V(x_n) + W(x_n - x_{n-1}) \quad , \quad (1)$$

where  $x_n$  is the absolute coordinate of the  $n$ -th particle. The corresponding dynamical equations are

$$m \ddot{x}_n + V'(x_n) + [W'(x_n - x_{n-1}) - W'(x_{n+1} - x_n)] = 0, \quad n \in \mathbb{Z}. \quad (2)$$

In order to investigate interstitial mobility we have chosen a cosine potential with the lattice period  $a$

$$V(x) = \frac{a^2}{4\pi^2} [1 - \cos(2\pi x/a)] \quad , \quad (3)$$

as the simplest, periodic substrate potential, with the linear frequency normalized to unity  $\omega_0 = \sqrt{V''(0)} = 1$ .

For the interaction between particles, we have selected the Morse potential

$$W(x) = \frac{C}{2b^2} [e^{-b(x-a)} - 1]^2, \quad x > 0. \quad (4)$$

which has a minimum at the lattice period  $a$  and a hard part that prevents particles from crossing. The well depth of this potential is  $C/2b^2$  while  $b^{-1}$  is a measure of the well width. Its curvature at the bottom is given by  $C = W''(a)$ , so that we can modulate the strength of the interaction without changing its curvature by varying parameter  $b$ .

In this system, an interstitial atom is represented by a doubly occupied well of the periodic potential (see the stable equilibrium configuration in panel (a) of Fig. 1). The relative coordinate of each particle with respect to its equilibrium position can be written as  $u_n = x_n - na$ . Using these relative coordinates, the interstitial

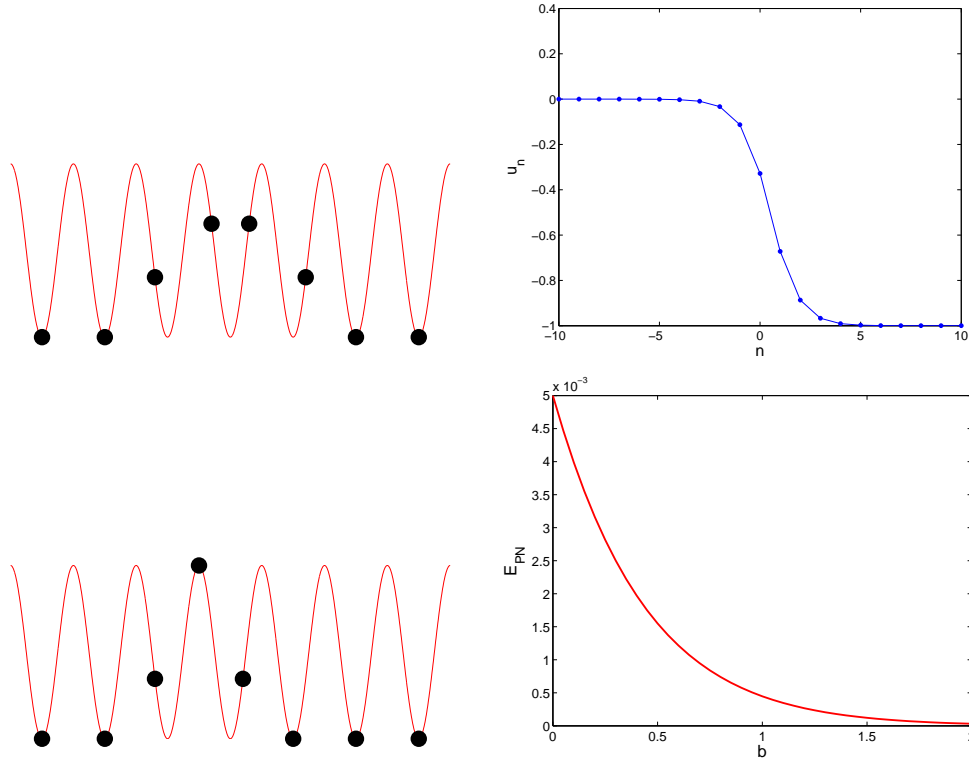


FIGURE 1. (a) Scheme of the stable equilibrium state of the Frenkel-Kontorova model with cosine substrate potential and Morse nearest neighbor interaction. The doubly-occupied well represents an interstitial. (b) Antikink corresponding to the stable equilibrium configuration in relative coordinates for  $b = 1$  and  $C = 0.5$ . (c) Unstable equilibrium configuration. (d) Peierls-Nabarro barrier for the antikink.

can be visualized as an antikink [2, 3]<sup>1</sup> as it is shown in panel (b) of Fig. 1. It is well-known that an antikink can be put into movement as soon as an energy barrier, the so-called Peierls-Nabarro barrier (PNB), is overcome. The PNB can be calculated as the energy difference between the unstable and stable antikink equilibrium configurations (panels (c) and (a) of Fig. 1 respectively) and decreases monotonically with  $b$  (see panel (d)).

It is worth noting that a vacancy can be visualized as a kink in relative coordinates. Its PNB increases with the parameter  $b$  and is always higher than the PNB of an interstitial, except for  $b = 0$  where both activation energies coincide. This is in accordance with the experimental fact that diffusion of interstitials is faster than that of vacancies, and support the idea that it is necessary to consider a nonlinear interaction potential in order to study diffusion of defects, since  $b = 0$  represents the linear limit of the Morse potential.

<sup>1</sup>Notice that in Ref. [3] the terms kink and antikink are interchanged.

In our F-K chain, stationary discrete breathers can be numerically obtained using the standard method of continuation from the anticontinuous limit [32, 33]. Translational motion of discrete breathers can be induced [34, 35] by adding a perturbation  $\vec{v} = \lambda(\dots, 0, -1/\sqrt{2}, 0, 1/\sqrt{2}, 0, \dots)$  to the velocities of the stationary breather, with the nonzero values at the neighboring sites of the initial breather center. The resulting DB kinetics is very smooth and resembles that of a classical free particle. Therefore, the total energy of a moving discrete breather can be estimated as the sum of its vibrational internal energy, equal to that of the stationary breather, plus its translational energy, which is equal to the energy of the added perturbation  $K = \lambda^2/2$ .

**3. Numerical study.** In order to investigate interstitial mobility, we have generated a breather centered at site  $n = -25$ , relatively far from an interstitial whose leftmost particle is located at  $n = 0$ , and then launched that breather towards it following the depinning method mentioned above. Throughout the paper, we have normalized the lattice period  $a$  and masses to unity and have taken  $C = 0.5$  so that moving breathers (MBs) exist in the system for a breather frequency  $\omega_b = 0.9$ .

As a result of the scattering the defect can be put into movement leading to long-range transport. We have found three well-differentiated regimes depending on the strength of the interaction potential. Below a critical value  $b \approx 0.83$  the result of the scattering is unpredictable. The dynamics is extremely sensitive to initial conditions (value of the perturbation  $\lambda$  and initial position of the breather) and the interstitial can travel or make random jumps (backward or forward) or even remain at rest. However, a net backward movement of the defect is only possible if the interaction potential is strong enough. In fact we have observed it only for values of  $b \lesssim 0.69$ . An example of a backwards travelling interstitial is shown in Fig. 2, whereas Figs. 3 and 4 show a backwards and forwards, respectively, hopping interstitial. In this case, the interstitial, after several random jumps, remains pinned on the lattice. These three figures display three panels. Left panel corresponds to an energy density plot where lines join points with the same energy in time while darker color indicates larger energy. Central panel displays the time evolution of the antikink (interstitial) center of mass. This graph helps to visualize more clearly the jumps of the interstitial particle and the final oscillatory state around an equilibrium configuration. Finally, right panel shows a streak plot with the time evolution of the breather and the interstitial. It is noteworthy that in our numerical experiments smaller values of  $b$  enhance backward movement and hopping behaviour of the interstitial particle. This latest behaviour is the only observed in the harmonic limit of the interaction potential ( $b = 0$ ).

Notice that the complexity of the dynamics is linked to the discreteness of the F-K model considered [36, 37]. In the continuous limit with  $b = 0$  the breather-antikink interaction is an integrable and well-known case, and the resulting scenario is quite simple: the breather always crosses the antikink which moves backwards during a brief lapse of time [38].

Due to the existence of an activation energy to move an antikink in the discrete case, interstitial motion is only found above a threshold value,  $K_c$ , of the kinetic energy of the incident breather. In the chaotic regime,  $b \lesssim 0.83$ , this threshold value, plotted in figure 5, increases monotonically in contrast with the PNB behavior found in the previous section. On the contrary, for  $b \gtrsim 0.87$  we find the opposite tendency:  $K_c$  decreases with  $b$  indicating a deep change in the dynamics. Indeed in

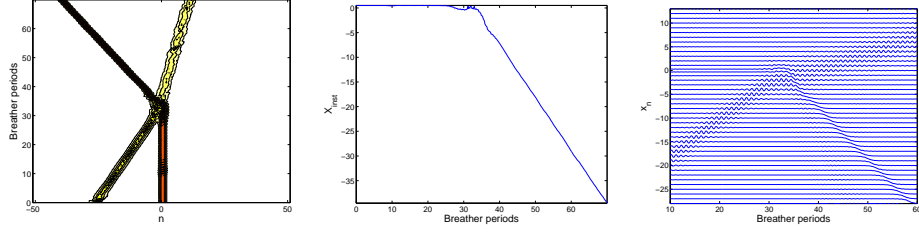


FIGURE 2. (Left panel) Energy density plot, showing a backward movement of the interstitial defect after breather scattering. The lines join points with the same energy in time. The darker colour the larger energy. (Central panel) Time evolution of the antikink energy center. (Right panel) Streak plot. Parameters:  $K = 0.0220$  and  $b = 0.5$ .

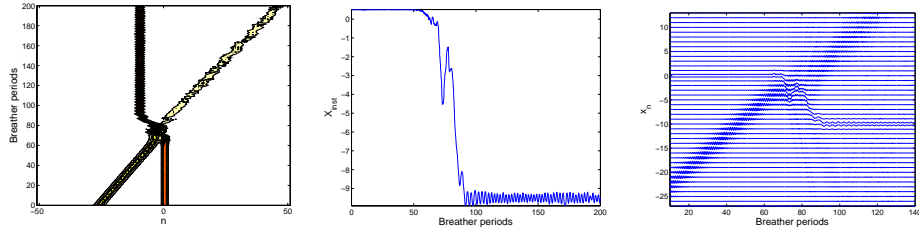


FIGURE 3. Same as Fig. 2 but for a hopping interstitial with net backwards displacement. Parameters:  $K = 0.0050$  and  $b = 0.2$ .

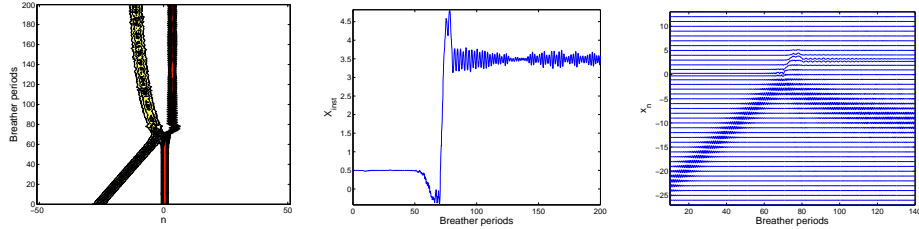


FIGURE 4. Same as Fig. 2 but for a hopping interstitial with net forward displacement. Parameters:  $K = 0.00605$  and  $b = 0.1$ .

this parameter regime, for  $K > K_c$ , the interstitial always moves forward after the scattering and, remarkably, it always moves with approximately constant velocity. In this regime, the Morse potential becomes essentially “flat” with a hard core and the dynamics is dominated by the repulsive part of the interaction potential. An example can be observed in Fig. 6. After the collision with the breather, interstitial motion is clearly linear in time. Its velocity has been computed fitting the points of the central panel with linear regression. In the transition between both regimes, i.e. for  $0.83 \lesssim b \lesssim 0.87$ , the interstitial always remains pinned on the lattice, at least for those values of  $\lambda$  for which the breather propagates without significant distortion.

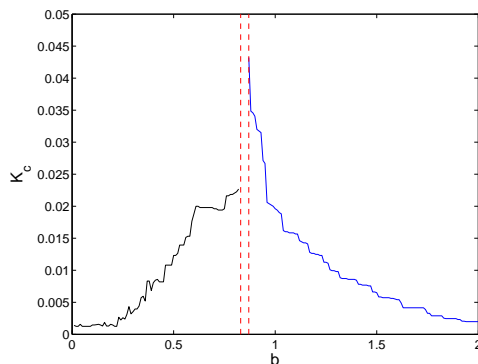


FIGURE 5. Minimum translational energy ( $K_c$ ) of the incoming breather needed to move an interstitial. In the band  $0.83 \gtrsim b \gtrsim 0.87$  the interstitial always remains pinned on the lattice.

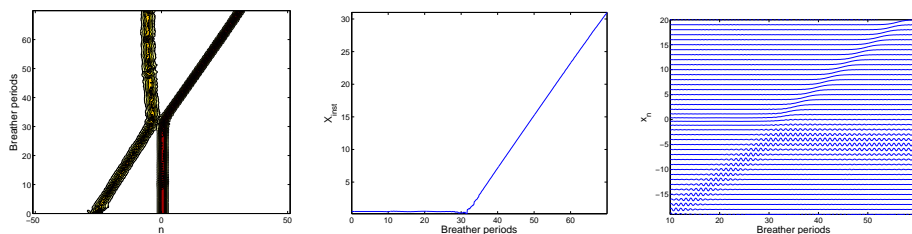


FIGURE 6. Same as Fig. 2 but for a breather with  $K = 0.020$  and  $b = 1.5$ . The interstitial always moves forward with constant velocity in the parameter region  $b \gtrsim 0.87$ ,  $K > K_c$

Fig. 7 shows the evolution of a pinned interstitial for  $b = 1$ . In this case the incident breather possesses a translational energy smaller than the critical value  $K_c$  and, consequently, the interstitial acts as a wall which totally reflects the breather. It is observed that, after the collision, part of the breather energy is employed in exciting an internal mode of the interstitial with a frequency smaller than that of the incident breather. This linear localized mode corresponds to the line below the phonon spectrum shown in Fig. 8 for the interstitial stable equilibrium configuration. Note that nonlinear localized modes do not exist close to the interstitial since the interaction potential is soft, and the frequency of the linear localized mode is always below  $\omega_b = 0.9$ .

As mentioned above, for  $b \gtrsim 0.87$  a stable interstitial propagating mode appears if the kinetic energy of the incident breather is higher than the threshold value  $K_c$ . In this parameter region the Morse potential becomes essentially a repulsive potential. In fact, in the limit  $b \rightarrow \infty$  it becomes a hard-sphere potential. For this reason, in this dynamical regime interstitial particles move roughly like hard spheres on a wavy energy landscape. After the breather scattering, the interstitial particle surmounts the energy barrier of the on-site potential well and collides with the particle that occupies the following well transferring its energy and momentum to it. In this way the defect propagates at constant velocity forever. In figure 9 we

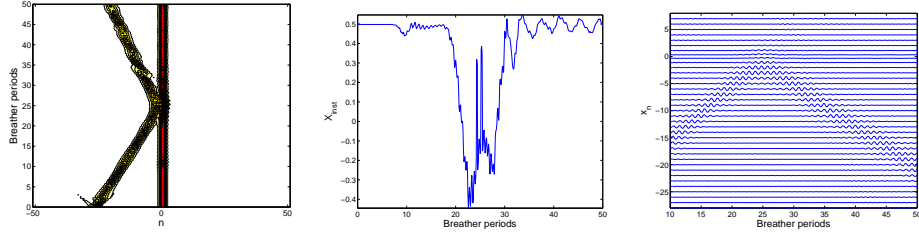


FIGURE 7. Same as Fig. 2 but for a breather with  $K = 0.0162 < K_c$  and  $b = 1$ . As the kinetic energy of the incident breather is below the threshold value  $K_c$ , the interstitial remains pinned on the lattice.

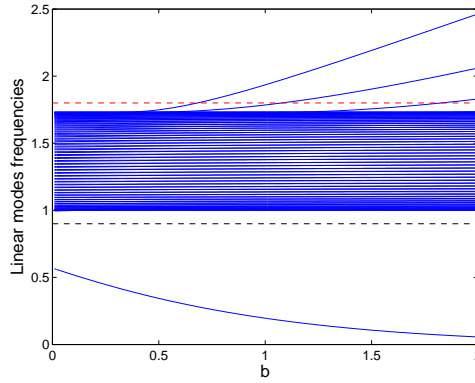


FIGURE 8. Linear modes spectrum of the stable equilibrium configuration for  $C = 0.5$ .  $\omega_b$  and  $2\omega_b$  are depicted through dashed lines.

have plotted the dependence of the velocity of this propagating mode on the kinetic energy of the incident breather. One can observe that just above the threshold energy, interstitial velocity increases with the kinetic energy,  $K$ , of the incoming breather. However for higher values of  $K$  the interstitial velocity tends to saturate around a value  $0.14 \frac{2\pi}{\omega_b} \approx 1$  site on the chain per breather period, independently of the coupling strength.

This phenomenon is confirmed in figure 10 where we have plotted the interstitial velocity versus parameter  $b$  for a fixed value of  $K$ . Indeed, for  $K = 0.045$  (dashed line) well above the energy threshold, interstitial velocity takes roughly the saturation value 0.14 independently of the coupling strength. Intermediate values of kinetic energy as  $K = 0.02$  (continuous line) also leads to saturation velocities independently of  $b$  but with values lower than 0.14 and less fluctuations.

**4. Conclusions.** We have presented numerical results arising from the interaction between a moving discrete breather and an interstitial defect in a FK chain. The main result is the existence of three differentiated regimes depending on the strength of the interaction potential. When the interaction between neighbors is strong the



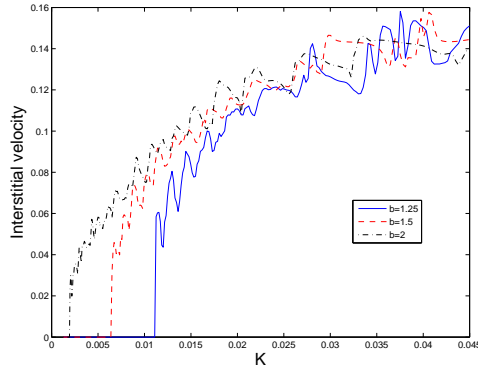


FIGURE 9. Interstitial velocity as a function of the translational energy  $K$  of the incident breather for three different values of the coupling strength in the regime ( $b \gtrsim 0.87$ ). In this regime the interstitial always moves forward with constant velocity because the interaction potential reduces essentially to a repulsive hard core.

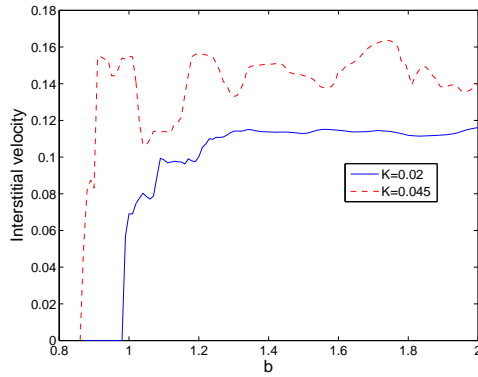


FIGURE 10. Interstitial velocity versus coupling strength for a fixed translational energy of the incident breather.

dynamics is chaotic and the behavior of the interstitial particle is unpredictable: it can jump backwards, forwards or remains at rest. However, if the interaction potential is weak enough, the defect moves forwards along the lattice with constant velocity. This stable propagating mode had not been observed to our knowledge in previous numerical studies concerning the interaction between moving breathers and point defects. The effect is ascribed to the fact that the interaction potential reduces essentially to a repulsive hard core. Between these two dynamical regimes there is a narrow intermediate range of the coupling strength in which the interstitial always remains pinned.

Out of that pinned regime, the kinetic energy of the incoming breathers must surpass a threshold in order to move the interstitial. This energy threshold has a non-monotonic behavior. It grows with parameter  $b$  in the chaotic regime, but decreases with  $b$  when the system losses sensitivity to initial conditions and the

propagating mode emerges. With due caution these results can assist in understanding the interaction of mobile discrete breathers with true initially stationary interstitial atoms lying adjacent to a chain in a crystal, which may be of the same or different species from that of the chain. The experiments reported in Refs. [26] and [27] are of each type. In these experiments an incident discrete breather must supply both the kinetic energy and the momentum of the interstitial that is put into motion. Moreover, once set in motion the interstitial, and thus its influence on the adjacent chain, is expected to move at the same speed as the discrete breather, thus carrying the defect as opposed to repeated sweeping by subsequent discrete breathers, which is less probable.

Our results are also in accordance with the experimental fact that interstitial defects diffuse easily and faster than vacancy ones, and support the hypothesis that scattering with high energy mobile breathers may play an important role for defect diffusion in crystals under ion bombardment.

**Acknowledgements.** Two of the authors (JC and BSR) acknowledge sponsorship by the Ministerio de Ciencia e Innovación (Spain), project FIS2008-04848.

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Received xxxx 20xx; revised xxxx 20xx.

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